November 2004

Science Technology

National Nuclear Security Administration's Lawrence Livermore National Laboratory

Probing the Universe

Also in this issue:

- Visualization Tools Improve Data Analysis
- Selecting an Explosive Yield
- New System for Quantifying Cellular Processes

About the Cover

Livermore has partnered with other researchers to build the balloon-lifted High Energy Focusing Telescope (HEFT), which will focus and measure x rays emanating from supernova remnant Cassiopeia A. As the article beginning on p. 4 describes, HEFT's focusing optics will provide dramatic improvements in sensitivity and angular resolution over previous instruments. In recent years, Livermore researchers have developed optics than can focus high-energy x rays for a variety of applications, including medical imaging, laser target characterization, and radiation detection. The cover image of Cassiopeia A is courtesy of the National Aeronautics and Space Administration, Chandra X-Ray Observatory, Goddard Space Flight Center, and authors U. Huang, et al. Also shown on the cover is an assembly of 72 mirror shells used for each of HEFT's three telescopes.



About the Review

Lawrence Livermore National Laboratory is operated by the University of California for the Department of Energy's National Nuclear Security Administration. At Livermore, we focus science and technology on ensuring our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published 10 times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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Prepared by LLNL under Contract No. W-7405-Eng-48



Lawrence Livermore National Laboratory

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S&TR, a Director's Office publication, is produced by the Technical Information Department under the direction of the Office of Policy, Planning, and Special Studies.

S&TR is available on the Web at www.llnl.gov/str.

Printed in the United States of America

Available from National Technical Information Service U.S. Department of Commerce 5285 Port Royal Road Springfield, Virginia 22161

UCRL-TR-52000-04-11 Distribution Category UC-99 November 2004

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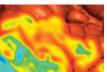
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Dedication of the Biodefense Knowledge Center

A national center to assist Department of Homeland Security (DHS) officials in the fight against bioterrorism has been established at the Laboratory. The Biodefense Knowledge Center (BKC) was dedicated September 10, 2004, during a visit to Livermore by DHS Under Secretary for Science and Technology Charles McQueary.

According to the new center's director, Livermore biomedical engineer Bill Colston, the BKC "will integrate what we know about biodefense and work to anticipate and respond to bioterrorist attacks." The BKC will draw on about 75 researchers based at four national laboratories—Oak Ridge, Pacific Northwest, Sandia, and Lawrence Livermore. Collaborators will also include three DHS University Centers of Excellence—the University of Minnesota, the University of Southern California, and Texas A&M University.

The new biodefense center will serve a number of functions. Initially, the center will provide assessments and respond to information requests from the DHS Operations Center, although other federal agencies may be able to use the center as a resource in the future. Another function of the BKC will be to integrate many types of information about biodefense. Among the data to be collected are the genome sequences for pathogens of concern, the existence and location of vaccines, the location of agent sequences for bioforensic attribution, and information about individuals, groups, or organizations that might be developing these pathogens. A third function of the BKC will be to prepare threat assessments for the DHS about potential bioterrorism attacks.

Contact: Bill Colston (925) 423-0375 (colston1@llnl.gov).

Optical sensor ready for commercialization

Graduate students at Syracuse University College of Law's Technology Transfer Research Center recently collaborated with Livermore employees from the Industrial Partnerships and Commercialization Office (IPAC) to market the six-degrees-offreedom (SixDOF) sensor to the commercial sector. The sensor attaches to computer-controlled machines, enabling them to operate in all six degrees of freedom. (See *S&TR*, October 1996, pp. 20–21.)

Former Laboratory mechanical engineer Charles Vann invented the SixDOF sensor in 1996, after he modified the design from a National Ignition Facility proposed alignment and diagnostic system. When the sensor was first created, the market was not developed enough to provide high demand for this

innovative technology. However, Norma Dunipace, partnership development manager for IPAC, says, "robots now have the brainpower and mechanics for this market to be profitable."

After an engineering prototype was developed, Dunipace and her group collaborated with Theodore Hagelin, director of New York State Science and Technology Law Center, and his team of graduate students at Syracuse University. Alex Padanyi, a research assistant from Syracuse who worked on the commercialization report, was a summer scholar in IPAC, helping to design a more thorough marketing strategy to obtain commercial licenses for the sensor. Dunipace foresees obtaining a license in the next year. *Contact: Norma Dunipace (925) 422-5995 (dunipace1@llnl.gov).*

Cleaner combustion with direct carbon conversion

Direct carbon conversion is an electrochemical process that converts carbon particles obtained from different fossil fuels directly into electricity without the need for such traditional equipment as steam-forming reactors, boilers, and turbines. The technology, which has been demonstrated in small-scale tests, would push the efficiency of using fossil fuels for generating electricity much closer to theoretical limits than ever before. The work is the result of a four-year study funded by Livermore's Laboratory Directed Research and Development Program.

Chemist John Cooper, a scientist in the Chemistry and Materials Science Directorate, says the method "would reduce carbon dioxide emissions, which are largely responsible for global warming, by producing a pure carbon dioxide byproduct that could be sequestered or used in industry at no additional cost of separation or concentration." If proven successful and adopted on a large scale, the process could conserve fossil resources by allowing more power to be harnessed from the same amount of fuel, while cutting the amount of carbon dioxide produced per kilowatt-hour almost in half.

"Direct carbon conversion has the potential to be the long-sought 'clean coal' technology," says Cooper. The new technology uses particles of elemental carbon whose atoms exhibit a high degree of structural disorder. These particles are wetted by a mixture of molten lithium–sodium and potassium carbonate at a temperature of about 750°C. The material reacts with carbon and oxygen from the ambient air to form carbon dioxide and electricity. Cooper says the reaction yields 80 percent of the carbon–oxygen combustion energy as electricity. It provides about 1 kilowatt of power per square meter of cell surface area—a rate high enough for practical applications.

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Focus on High-Energy Detection

AWRENCE Livermore has partnered with the California
Institute of Technology (Caltech), Columbia University, and
the Danish Space Research Institute to launch the High Energy
Focusing Telescope (HEFT), a balloon-borne mission that will
demonstrate a new capability to image hard x rays from black holes
and other exotic objects in the high-energy universe. Researchers
at the Laboratory expect the results from HEFT to provide new
information about deep space.

The HEFT mission, sponsored by the National Aeronautics and Space Administration, is testing new telescope optics and detectors developed at Livermore and Caltech. If successful, the telescope's groundbreaking technologies may be slated for a future satellite observatory. Livermore scientists used a grant from the Laboratory Directed Research and Development Program to upgrade the gondola that carries the telescope to enable a unique science return from the instrument. The experiment's goal is to map out the distribution of high-energy emissions from titanium-44 in the supernovae remnant Cassiopeia A. These data would shed light on the nucleosynthesis of elements essential to life, including calcium, and on the nature of the supernova explosion itself.

The HEFT telescope makes use of both the Laboratory's advances in the design and fabrication of hard x-ray focusing optics and Caltech's development of detector materials to solve the problem of collecting and analyzing hard x rays from very weak sources. The Laboratory is also adapting the technologies used to study astrophysics phenomena in the universe to advance the development of radiation detection equipment needed to protect the nation from nuclear terrorism.

The problem of finding nuclear material that may be covertly transported or hidden by terrorists is one of the "grand challenges" of homeland security. While the solution will almost undoubtedly involve a highly coordinated system of sensor and intelligence capabilities, the principal means of detecting and identifying nuclear materials is by their distinctive hard x radiation. Therefore, significant advances in x-ray detection science and technology have a direct and invaluable application to the nuclear terrorism problem.

As described in the article beginning on p. 4, the detectors developed for HEFT can be applied to countering nuclear terrorism. The cadmium–zinc–telluride devices replace standard germanium detectors that must be cooled to –200°C to operate. Eliminating the cooling requirement by using these room-temperature devices results in compact, high-resolution sensors that can be easily packaged as versatile, portable radiation detectors for first responders.

Because of the many years the Laboratory has worked with its partners in its high-energy astrophysics programs, the HEFT technology was ready to contribute to the needs of homeland security in the aftermath of September 11, 2001. Long-term basic research and collaborations with partners in areas that share science and technology with Livermore's missions are essential to our ability to respond to the nation's evolving national security needs.

■ William H. Goldstein is associate director of Physics and Advanced Technologies.

Probing the Universe with Mirrors That Trick Light

High-energy focusing optics are providing scientists with new information about deep space.

OR astrophysicists, stargazing may be different than for most people, who are content to admire a star's beauty or possibly make a wish. More than a few astrophysicists wish they could be closer to the stars—or to at least have more sophisticated probing instruments—to understand more about the universe. Astrophysicists study x rays originating from our Sun, stars, and supernova remnants to understand the extreme physical processes occurring there.

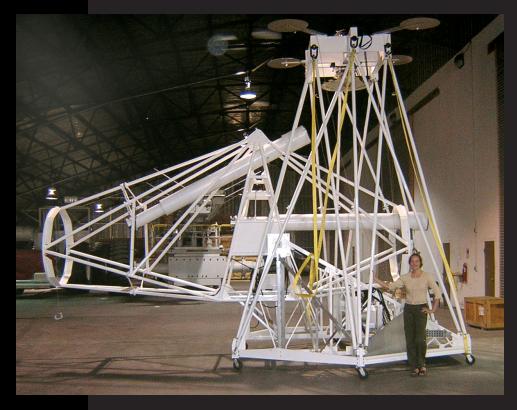
In recent years, Livermore researchers have developed optics for astrophysical applications that can focus hard x rays (that is, x rays with energy levels above 20 kiloelectronvolts) emanating from celestial objects, such as supernovae. In addition to astrophysics, hard x-ray optics have a variety of possible applications, including medical imaging, laser target characterization, and radiation detection.

Livermore researchers have long contributed to advancements in supernova astrophysics because studying thermonuclear processes is a central part of the Laboratory's national security mission, and the physical processes involved in a nuclear weapon and an exploding star are similar.

Livermore physicist Bill Craig, who is involved in several projects using x-ray optics, says, "We can do a better job of detecting illicit radioactive sources because of what we have learned from our developments in astrophysics. Whether the radiation source is from a black hole in space or nuclear material in a dirty bomb, detecting the source involves the same challenge, which is to pick up faint signals (high-energy photons) amidst background radiation."

Up, Up and Away

Recently, Livermore partnered with the California Institute of Technology (Caltech), Columbia University, and the Danish Space Research Institute (DSRI) to build the High Energy Focusing Telescope (HEFT), which was awaiting a balloon-launch into Earth's atmosphere at press time. The telescope uses optics that provide a dramatic improvement in sensitivity and angular resolution over previous instruments and allow scientists to observe hard x rays emitted



The High Energy Focusing Telescope uses three high-energy x-ray focusing optics modules and cadmium–zinc–telluride detectors to observe some of the most energetic objects in space.

by some of the most energetic objects known, including supermassive black holes, stars, and pulsars. (See the box on p. 6.) Livermore researchers are most interested in measuring x and gamma rays of titanium-44, a radioactive isotope of titanium produced in supernovae.

Researchers are interested in titanium-44 because it is formed at the mass cut, the boundary between material that is ejected from a supernova and the material that is captured by gravity and forms a neutron star. The mass-cut region provides the deepest possible view into the details of the supernova explosion. Craig says, "Because we know titanium-44 has a half-life of approximately 80 years, we can look at the distribution of titanium-44 and learn more about what happened at the time a star exploded." All of the calcium in our bodies also comes from the decay of titanium-44 in supernovae, an interesting irony considering titanium is often a surgeon's material of choice when replacing damaged bones. HEFT will focus on Cassiopeia A, a supernova

The Electromagnetic Universe

The entire range of light energies, including what humans can and cannot see, is called the electromagnetic spectrum. The range includes (from lowest to highest energy level) radio waves, microwaves, infrared, optical, ultraviolet, x rays, and gamma rays. Researchers describe the types of electromagnetic radiation by energy, wavelength, or frequency. The name distinctions are due to the vast differences in energy between the types and provide researchers with a practical way to reference them.

Light acts like both a particle and a wave and comes in discrete amounts—the least being a simple photon. Low-energy photons, for example radio waves, tend to behave more like waves, while higher energy photons, such as x rays, behave more like particles. These differences affect how researchers build instruments to measure photons. Celestial gamma and x rays are most accurately measured above Earth's atmosphere because they are absorbed as they travel through the atmosphere.

When scientists observe the sky at low x-ray energies (0.25 kiloelectronvolt), they see a glow from the radiation emitted from hot gas that fills some of the space between the stars. Because of the galaxy's shape, radiation from within it is brighter in some directions and dimmer in others. When scientists observe the sky at higher x-ray energies (above 0.50 kiloelectronvolt), the background radiation appears isotropic; that is, it looks the same in all directions. As a result, scientists believe that higher-energy x rays come from outside the galaxy.

A variety of celestial objects also emit x rays, including single stars, binary star systems, supernova remnants, galaxies, clusters of galaxies, and active centers of galaxies (active galactic nuclei, or AGN). X rays usually come from very hot gaseous matter (millions of kelvins) or from very fast electrons losing their kinetic energy. AGNs emit both x and gamma rays. Because AGNs can undergo changes in much less than 1 second, researchers study them at all wavelengths. X rays emitted from AGNs can provide scientists with insights into the physical processes occurring there.

remnant that appears to be 327 years old. (The distance to Cassiopeia A from Earth is approximately 10,000 light years, so the star's explosion actually occurred more than 10,300 years ago.)

With funding from Livermore's Laboratory Directed Research and Development Program, Livermore also developed the technology that was used for building the gondola to hold HEFT's optics. "Building the gondola was a challenge because we had a 1,400-kilogram instrument suspended from a balloon as big as a football stadium," says Craig. "The gondola has to hold this instrument steady at an altitude of 40 kilometers to lock the telescopes onto a source with a precision equal to three times the width of a human hair." The HEFT team also built star trackers that can lock onto stars during the day or night to accurately ascertain the position of the gondola and point the optics toward an x-ray source.

X rays are photons with energy levels that range from approximately 0.1 to 100 kiloelectronvolts. (For comparison, visible light has an energy level of 0.002

to 0.003 kiloelectronvolt.) Energies in the lower end of the range are called soft x rays, and those in the higher end are called hard x rays. Measuring x rays from the Earth's surface is impossible, because they are mostly absorbed by Earth's atmosphere. Instead, detectors must be deployed at an altitude that places them above 99 percent of the atmosphere.

In 1995, Livermore helped launch the Gamma Ray Arcminute Telescope Imaging System (GRATIS), which was one of the first high-altitude balloons to carry a high-energy imager. The optics system consisted of 36 coded-aperturebased telescopes. In a coded-aperturebased telescope, an image of the source is encoded on a detector by placing a sheet pierced with a hole pattern in front of the detector. The holes in the mask project a pattern on the detector so that the direction of the incoming photons can be inferred. The GRATIS balloon reached an altitude of 40 kilometers and remained aloft for 36 hours. GRATIS tracked a number of astronomical gamma and x-ray sources, including the center of our galaxy, a prime black hole candidate (Cyg X-1), and an unusual x-ray binary system (Cyg X-3).

Craig notes that both coded-aperture-based systems, such as the one used for GRATIS, and focusing optics-based systems are valuable, depending on the application. "If we want to view the whole sky at once, a coded-aperture-based system is best. But if we need to focus on one specific area and learn as much as we can about it, focusing optics are much better, increasing sensitivity by as much as a factor of 1,000 over coded-aperture-based systems."

In addition to the interference from Earth's atmosphere, another challenge when measuring x rays is they don't reflect off an optic's glass surface in the same way that visible light does in traditional telescopes. Because of their high energy, most x-ray photons will penetrate the mirrors and be absorbed if they approach at a perpendicular angle. At this angle, no photons would be reflected onto the detectors that measure their position and energy. Researchers found that for high-energy focusing

optics, they must design mirrors nearly parallel to incoming x rays to maximize the reflected light. In this configuration, the photons glance off the surface of the mirrors, in much the same way a stone is thrown to skip over water. The critical graze angle (the maximum incidence angle at which reflection can occur) is inversely proportional to the photon energy, so reflecting high-energy x rays requires very small incidence angles. For example, the critical angles for x rays emitted from iridium at energy levels of 1, 10, and 100 kiloelectronvolts are approximately 2.0, 0.6, and 0.1 degrees, respectively.

Focusing X Rays Where They Count

In 1952, German physicist Hans Wolter designed a nearly cylindrical mirror that increases collection efficiency and brings x rays to a common focus. Technology at the time prevented Wolter from accomplishing his goal to construct a short-wavelength microscope for

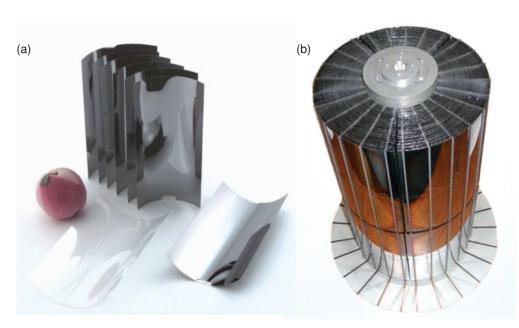
biological research. However, his design advanced the development of focusing optics for telescopes.

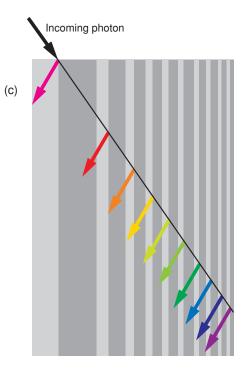
When focusing telescopes were first developed, they were limited to the soft x-ray band because of the technical challenges in extending grazing incidence x-ray optics to high energy and the limits in spatial resolution that existing hard x-ray detectors could achieve. Recent developments in multilayer optics and high-atomic-number (high-Z) solid-state pixel detectors now make both focusing optics and detectors possible at high x-ray energies. These advances provide improvements in sensitivity and resolution far beyond what are achievable with coded-aperture-based instruments.

HEFT collaborators found they could increase the optics' efficiency by collecting light from a larger aperture using a multilayer structure invented specifically for hard x-ray optics. A multilayer is a coating composed of

alternating layers of high- and lowatomic-number materials, such as molybdenum and silicon or tungsten and boron carbide. The varying thickness of the layers within the coating makes the design efficient for a wide range of angles and photon wavelengths (energies). "In a straightforward approach, we would have to add more glass-thousands of mirrors—to get the reflectivity to cover the emitting source area we need to measure," says Craig. "Instead, we looked at how we could change the critical graze angle. The multilayer approach works because it 'tricks' light into seeing a number of mirrors."

Each telescope on HEFT features Caltech's innovative detector system, which has two solid-state, cadmiumzinc-telluride pixel detectors, each with more than 1,000 pixels. A high-Z



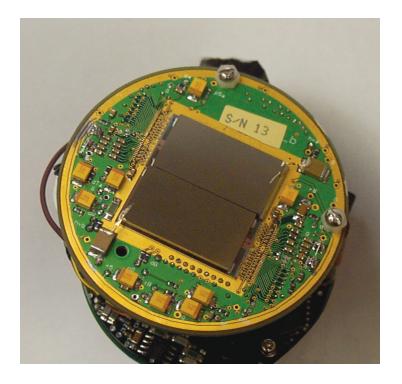


(a) The High Energy Focusing Telescope's (HEFT's) optic mirrors are made from glass originally developed for flat-panel computer monitors. The glass is thermally formed and then covered with a multilayer coating composed of alternating layers of materials that vary in thickness. (b) Seventy-two mirror shells are assembled for each of HEFT's three telescopes. (c) The multilayer structure is efficient for a wide range of angles and photon wavelengths (energies). Photons are reflected off the interface between the different materials, thus "tricking" light into seeing more mirrors. The colored arrows indicate the reflectivity from a range of x-ray energies, from the lowest (pink arrow) to the highest (violet arrow).

element, such as cadmium, increases a detector's sensitivity and spatial resolution because the large number of protons and neutrons in its nucleus makes it more efficient at stopping photons. In addition, each detector is bonded to a custom silicon chip that contains an amplifier with microelectronics for every pixel. Each 500- by 500-micrometer pixel can thus measure photon energy and spatial resolution.

Craig says, "In traditional systems, an external amplifier is connected to a detector. With those systems, we can measure the energy, but we can't be certain of its directional source because we don't know where on the detector the photon hit. And, if we subdivide the detector and increase the number of amplifiers to improve spatial resolution, we end up with a very large system that becomes impractical." The focusing optics system also dramatically limits background emissions from the atmosphere and high-energy cosmic-ray particles from interfering with the detector.

Each of the High **Energy Focusing** Telescope's three optic modules focuses x rays onto a solid-state detector. The detector consists of two pieces of cadmiumzinc-telluride, each of which is 2.6 by 1.3 centimeters wide and 2 millimeters thick. The large number of protons and neutrons in cadmium's nucleus make the material efficient at stopping photons.



Low-Cost Fabrication Techniques

Producing high-quality reflective optics can be expensive. For example, the National Aeronautics and Space Administration (NASA) spent \$700 million to make the four sets of mirrors for the Chandra X-Ray Observatory launched in 1999. The costly processing technique involved carving ceramic glass from a monolithic blank, and then polishing and measuring each mirror. Once the substrate was finished, a reflective coating was deposited on the interior of the optic. HEFT required 72 mirror shells on each of its three telescopes, so the cost to produce the mirrors using this method would have been prohibitive.

The HEFT team developed a new fabrication method that was comparatively inexpensive at \$100,000 per telescope. The process starts with a thin glass originally developed as a substrate for flat-panel displays on computer laptops. The inexpensive and high-quality glass is inherently smooth and eliminates the need for polishing, which is one of the most

labor-intensive steps in other techniques. The flat sheets are thermally formed into the appropriate shape and then covered with a thin multilayer. Small pieces of graphite are inserted between the mirrors to precisely position each mirror and provide space for the photons to reflect off the mirrors. Columbia University prepared the glass for HEFT, and a Livermore engineering team, led by Todd Decker, developed the assembly method.

Rising Above the Atmosphere

Telescopes launched into the atmosphere by balloon are relatively inexpensive compared with telescopes launched into space by satellites. However, the balloons can rise only 40 kilometers above Earth, and atmosphere above this height can interfere with measurements. In addition, the lifetime of helium-filled balloons is limited; they can float at the required altitude for only a day or two.

NASA is studying a proposal by the HEFT team to build the Nuclear Spectroscopic Telescope Array (NuSTAR), which will take a telescope for focusing high-energy x rays into space and above the atmospheric interference. NuSTAR will fly 525 kilometers above Earth's surface and stay in orbit for 3 years. It will be the first hard x-ray focusing telescope in space and will observe energies from 10 to about 100 kiloelectronvolts, providing a 1,000-fold increase in sensitivity over previous missions.

NuSTAR will survey galactic nuclei, observe the synthesis of elements in supernova remnants, and study high-energy blazers. NuSTAR's focusing optics will function similarly as they did for HEFT, but NuSTAR will have 130 nested mirror shells on each of its 3 telescopes. The HEFT team, in partnership with NASA's Jet Propulsion Laboratory, proposed building NuSTAR, and their proposal was selected in mid-2003 as one of five missions now engaged in a year-long competition for two flight opportunities as part of NASA's Small

Explorer Program. NASA plans to announce the two winning missions, which would launch in 2007 and 2008, in November 2004.

Adapting the Technology

Livermore's collaborative projects sometimes reap bigger dividends than planned when applications spin off in unexpected directions. For example, the same technology Caltech used to build the detector system for HEFT has been adopted for use on RadNet, a Livermore-developed radiation detector for homeland security. (See *S&TR*, September 2004, pp. 4–11.)

In 2001, Craig and Simon Labov, director of Livermore's Radiation Detection Center (RDC), were discussing radiation detection requirements at an RDC workshop when Labov expressed the need for a handheld system that could run on batteries and be capable of high spatial resolution. Fresh from the collaborative effort on HEFT, Craig believed its detector technology could be applied to a handheld radiation detector. Caltech had not yet published data on its detector technology. However, Craig's collaborations on HEFT, and later with the RDC, spawned the needed technology to develop RadNet.

RadNet combines a cellular telephone, a personal digital assistant with Internet access, and a Global Positioning System locator with a radiation sensor. Because the instrument is inexpensive, first responders can take a number of them in the field to cover a wide geographic area. "It's amazing," says Craig, "how much of our work comes full circle. We're now using what we've learned from the detector technology in RadNet to build a larger array for the Energetic X-Ray Imaging Survey Telescope, another large NASA project to study black holes."

The \$30,000 Mouse

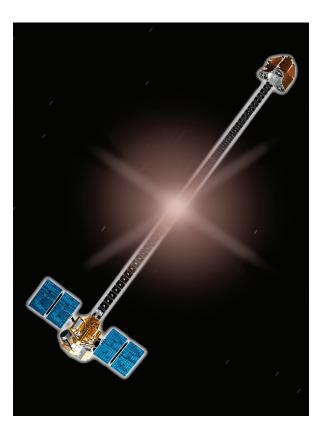
The Laboratory is also applying its x-ray optics expertise to medical imaging. Livermore physicist Michael Pivovaroff leads a team developing x-ray optics for

cameras to image mice used in research. The Small Animal Radionuclide Imaging System is funded through the Department of Energy's Office of Biological and Environmental Research and the Campus-Laboratory Collaborations Exchange Program administered by the University of California (UC) Office of the President. The project brings together researchers from Livermore, UC San Francisco and Berkeley, NASA's Marshall Space Flight Center, and DSRI.

Advances in transgenic manipulation (altering the genome of a species by introducing a gene or genes of another species) have allowed researchers to produce genetically engineered mice with human diseases. By creating and analyzing animals that harbor a known condition or planned changes in genes, biomedical researchers can observe how effective a treatment is or how well a drug controls DNA damage or carcinogenesis. Each of

these mice can cost as much as \$30,000. They hold tremendous promise to help solve human health problems.

Nuclear medicine studies of animals and humans currently rely on singlephoton emission tomography or positron emission tomography. These collimatorbased imaging techniques are limited to spatial resolutions between 1 and 2 millimeters. However, many research problems can be addressed only with a resolution of about 100 micrometers, which is 10 times finer. Also, because a single cell measures just tens of micrometers across, waiting for a tumor to reach the 1-millimeter size required by conventional imaging techniques prevents researchers from studying the critical first stages of tumor development. With current techniques, it would either be impossible or prohibitively expensive to construct an instrument with greater resolution.



The Nuclear Spectroscopic Telescope Array (artist's conception shown here) would be the first satellite mission with a high-energy x-ray focusing telescope in space and would provide a 1,000-fold increase in sensitivity over previous missions.

The Livermore team plans to increase the resolution to 100 or possibly 10 micrometers by bending the shape of the multilayer mirrors used for the telescope design and adapting them for use in a microscope. Pivovaroff says, "Limits in optical fabrication and coating techniques prevented Wolter from fulfilling his dream of constructing a shortwavelength microscope for biological research in the 1950s. Today, we have the technology to realize his vision."

This increase in resolution will allow in vivo assessment of biological and biomolecular interactions in mice and other small animals. It will also allow researchers to administer lower doses of radioisotopes, which will lessen the chance for the radioisotope to adversely affect results.

The Livermore team designed several biological optics systems using Monte Carlo simulations of optical designs and multilayer methods. One design for imaging iodine-125 consists of 102 nested mirror shells and can resolve up to 145 micrometers. Recent experiments with single-shell prototypes achieved the expected resolution and demonstrated that practical optics can be built with 10 times better resolution and efficiency than most pinhole collimators.

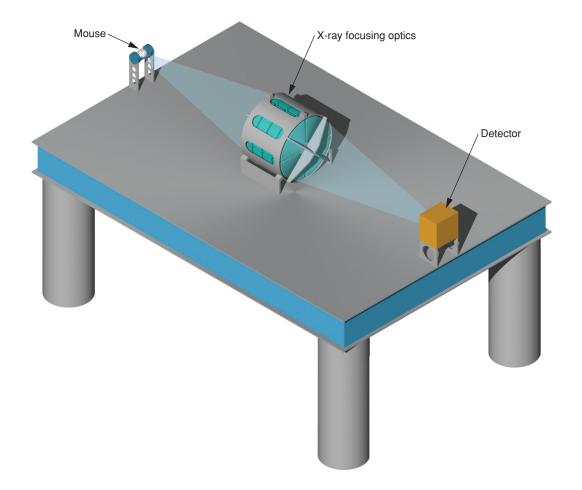
Verifying Targets

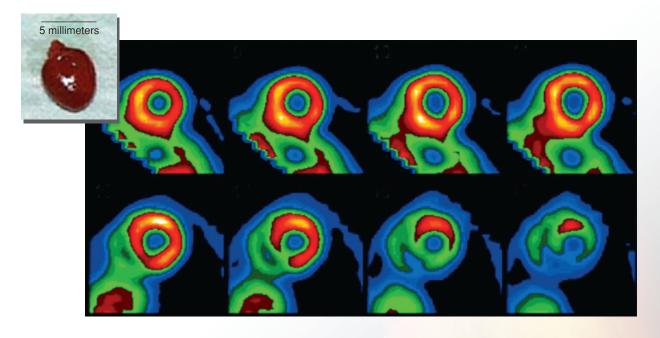
X-ray optics may also prove valuable for target characterization and imaging on experiments at the National Ignition Facility (NIF). Researchers need to be able to verify nondestructively that mesoscale

(the length scale between macro and nano) parts are assembled correctly. The parts must not be damaged before they become a component of an experiment. (See S&TR, October 2003, pp. 18–26.) Many techniques already exist to characterize objects, but they cannot image through high-Z materials.

NIF researchers also need to confirm their experimental results. For example, if they suspect that light will be emitted in a certain direction, they need an imaging tool that can measure it. One possible method is to use reflective optics to image x rays emitted during an experiment. Livermore's work on extreme ultraviolet lithography, of which multilayers are an important component, will contribute to improving

X-ray focusing optics are being adapted in a microscope design for the Small Animal Radionuclide Imaging System. In the design shown here, the optics will focus x rays emitted from a mouse that is injected with iodine-125 onto a detector.





This false-color image shows a mouse heart injected with an iodine-125 agent. In the tomographic reconstruction, the brighter colors correspond to more emission from that region of the heart wall. (Image courtesy of the University of California at San Francisco.)

the resolution of these systems and may, ultimately, lead to the development of diffraction-limited x-ray optics.

Fortunately, the bright stars we gaze upon reveal not only beauty but also a treasure trove of valuable information. The fact that the stars are actually a vision created thousands of years ago only adds to their allure and to the value of the information scientists can gather. As Livermore continues to explore thermonuclear fusion as part of its national security mission, Laboratory researchers can look upward for more answers from the stars.

-Gabriele Rennie

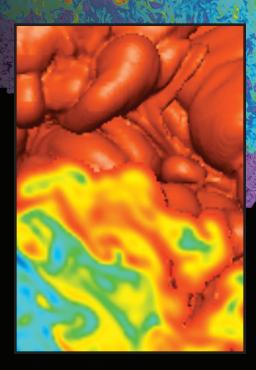
Key Words: Gamma Ray Arcminute Telescope Imaging System (GRATIS), hard x ray, High Energy Focusing Telescope (HEFT), multilayercoated mirrors, Nuclear Spectroscopic Telescope Array (NuSTAR), Small Animal Radionuclide Imaging System, x-ray optics.

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From Seeing to Understanding

Livermore computer
scientists are revolutionizing
the ways researchers
visualize enormous amounts
of supercomputer data.



Supercomputer simulations contain extraordinary amounts of detail. Livermore scientists are developing new methods for scientists to search images and locate the areas of interest. This image was generated on the Production Visualization Cluster—a visualization engine—using the MIRANDA code and Terascale Browser software. It depicts the instability of two fluids mixing together.

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three-dimensional (3D) supercomputer simulations play a major role in making sure the nation's nuclear stockpile remains safe and reliable. The simulations require supercomputers performing trillions of operations per second (teraops) often for weeks at a time.

Understanding these simulations depends, to a great extent, on the human eye to carefully scrutinize the vast amounts of simulation information translated into still and moving images. These images allow researchers to gain insight into how a nuclear weapon operates and the effects of aging on its many components. Livermore computer scientists are developing new ways to see and understand the latest simulations by combining inexpensive and ubiquitous microprocessors, graphics cards favored by video-game fans, and opensource software. These components are the heart of the powerful visualization engines that turn reams of data into practical 3D images and movies.

Livermore's supercomputers dedicated to stockpile stewardship are part of the Advanced Simulation and Computing (ASC) Program. An element of the National Nuclear Security Administration (NNSA), ASC is advancing supercomputing so scientists can make the much higher fidelity physics and engineering simulations needed to assess the safety, reliability, and performance of the nation's nuclear weapons stockpile.

The 12.3-teraops White machine, in operation since 2000, is Livermore's most powerful ASC supercomputer. Two new ASC computers, Purple and BlueGene/L, will be delivered in 2005 and housed in Livermore's new \$91-million Terascale Simulation Facility (TSF). Purple will fulfill the ASC Program's long-sought goal of developing a machine that operates at 100 teraops, considered the entry point for prototype high-fidelity, full weapons system simulations. BlueGene/L, a research and evaluation machine, will have a peak performance of 180 to 360 teraops.

Modern ASC supercomputers, such as White, Purple, and BlueGene/L, consist of thousands of nodes, each composed of 2 to 16 microprocessors. These machines perform what is known as massively parallel computing in which nodes work together on a problem. They are also scalable; that is, simulations can be done with a few nodes or the entire set, and nodes can be added to tackle more difficult problems. (See *S&TR*, June 2004, pp. 12–20.)

The latest generation of ASC machines generate enormous amounts of data that are sometimes the result of weeks of round-the-clock number crunching. Three-dimensional, time-varying data sets of tens of terabytes (trillions of bytes) are now common, and petabyte (about 1,000 terabytes) data sets are on the horizon. As a result, an urgent need exists to develop new ways to visualize vast quantities of numbers.

Transforming Visualization

Livermore's Visual Interactive
Environment for Weapons Simulation
(VIEWS) Program, part of the Laboratory's
ASC effort, is helping scientists visually
explore, manage, and analyze data from
advanced simulations. (See S&TR,
October 2000, pp. 4–12.) The program is
fulfilling a plan developed several years
ago to transform the way scientists look
at their data. This transformation is being
accomplished by adopting new visualization
computer architecture and developing
software and analytical tools to run on the
new hardware.

The VIEWS team's mantra is "see and understand." "Early on, when we were trying to display the results of our huge computer runs, the emphasis was on seeing a large amount of data at once," says computer scientist and VIEWS program leader Steve Louis. "We have progressed to displaying and managing the details of that data in high-resolution format."

Louis says the emphasis has shifted to *understanding* because "*seeing* only takes you so far. We want to make it easier to

find interesting regions in simulations and track those regions over time. We also want to visually compare a set of simulations or contrast data from a simulation with data from an experiment." The underlying goal is to support the ASC Program's vision of improved predictive capability for the performance of stockpile nuclear weapons and their components through experimentally validated simulation tools.

Currently, ASC supercomputers use visualization engines that turn the data produced by supercomputers into images displayed on individual computer monitors, larger-scale screens, or massive powerwalls. (See the box on p. 14.) These visualization engines and their systems software have until recently been supplied and integrated by commercial vendors. This approach worked well in the past, but it offers limited expansion capability because of the constraints of a shared-memory architecture. The processors and graphics cards used in the shared-memory architecture are proprietary and expensive.

Computer scientists use the term scalability to indicate the ability of a computer to handle larger and larger problems and data sets. "You can only scale so far with our present ASC visualization engines before the necessary hardware and time to run the simulations start getting very expensive," says Sean Ahern, a visualization project leader for VIEWS.

With an eye on the growing size of computer simulations, Livermore managers decided to transition from proprietary shared-memory visualization engines to groups or "clusters" of commercial personal computer (PC) microprocessors and highend graphics cards found in gaming boxes and many PCs. When combined with a high-speed network running on a Linux operating system and software tools written in open-source (not vendor-proprietary) code, the clusters outperform the larger and significantly more expensive proprietary engines. The clusters are also easily expandable by simply adding more units.

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A Closer Look at Clusters

Linux visualization clusters operate like modern supercomputers: They farm out problems in pieces to hundreds or thousands of microprocessors networked together and working in parallel. Clusters offer substantially more power in the same space—and at much less cost—than

the proprietary engines they replace. Individual cluster nodes typically have two microprocessors and one graphics card. These nodes have their own memories, in contrast to shared-memory designs.

The key to the visualization clusters' remarkable price—performance ratio is their high-end graphics cards containing

graphical processing units (GPUs). "The GPUs give us 10 times the performance for one-fifth the cost of cards found in previous ASC visualization engines," says Ahern. Specialized, 3D GPUs were once available only in expensive workstations. Linux clusters now use gaming GPUs that cost between \$300 and \$400, are

Getting the Big Picture

To see the results of their simulations, Livermore researchers use a variety of display devices ranging from relatively small desktop monitors to powerwalls. Powerwalls work by aggregating, or "tiling," the separate images from many projectors to create one seamless image. Large powerwalls exist in several Livermore buildings.

Powerwalls, which are typically the size of a conference room wall, allow a group of scientists to study still images or watch a movie, frame by frame. "Researchers can freeze images, pan, zoom,



Terascale Simulation Facility shows a simulation of results from an experiment mixing two liquids of different densities, which was conducted at the University of Arizona. Powerwalls work by aggregating, or "tiling," the separate images from many projectors (inset) to create one seamless image.

move back and forth in time, and see details too subtle or small to discern on a desktop monitor," says electronics engineer Bob Howe, head of infrastructure and facilities for the Visual Interactive Environment for Weapons Simulation (VIEWS) Program. At the same time, because of the powerwall's sheer size, users can still view the global problem while keeping the details in perspective. Powerwall displays are especially useful for presentations and formal reviews.

Livermore's new Terascale Simulation Facility (TSF) has two large powerwalls for major reviews and division meetings, one of which is used to display classified simulations in a room with removable seating for 130 people. A similar powerwall in a room with auditorium-style seating will be used for unclassified work. The TSF also has smaller powerwalls designed for more informal interactions.

Over the years, new products have been introduced to improve the resolution, clarity, and uniform brightness and color of powerwalls. Flexible screens have been replaced with hard, flat screens, and new projectors using digital-light-processing technology achieve higher contrast, greater brightness, and automated color balancing. For video delivery to powerwalls and other high-resolution displays, Howe is overseeing the transition from existing analog-based switching and delivery to newer digital technologies.

Some Livermore physicists have asked for stereoscopic capabilities to improve the three-dimensional (3D) information in powerwall presentations. Currently, 3D visualization is achieved by interactively shading and rotating an image to reveal the sides and details of objects slightly hidden behind foreground surfaces. Visualization experts plan to deploy active stereo technology, which uses high-frame-rate stereo projectors and requires viewers to wear shuttered goggles that repolarize about 45 frames per second per eye to minimize flicker.

Howe notes that although powerwalls have proven indispensable for presentations, scientists spend most of their time working in their offices alone or with a few colleagues. "Those scientists want larger displays and more pixels on their office machines, and we're working hard to provide that." Howe and other VIEWS visualization experts are keeping a close eye on new monitor and projector designs, many of which are beginning to enter the consumer market.

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powerful computers in their own right, and can calculate 100 billion operations per second (gigaops). Ever more powerful GPUs are announced every few months, and industry experts predict that videogame machines will contain GPUs capable of 1 teraops by 2006.

"Several years ago, we began watching the graphics cards appearing in PCs and gaming boxes. They didn't have the performance we need, but we could see where the cards were heading," says Louis. He notes that Livermore computer scientists, who were used to working closely with manufacturers in developing new computers and components, are now largely spectators in the multibillion-dollar gaming-hardware industry. Nonetheless, they have no objections to taking advantage of the hardware advances.

Paving the Way

The first Linux visualization cluster deployed at Livermore was the Production Visualization Cluster (PVC). PVC was designed to support unclassified applications on the 11.2-teraops Multiprogrammatic Capability Resource (MCR) machine and is being expanded to support the 22.9-teraops Thunder cluster supercomputer. With 64 nodes, each consisting of two processors and a graphics card, PVC went online in 2002.

By all measures, PVC has been highly successful. It is handling data sets of 23 terabytes to create animations involving 1 billion atoms. PVC generates these animations in about one-tenth the time and at one-fifth the cost of proprietary visualization engines, while simultaneously driving high-resolution displays in conference rooms and on powerwalls.

"PVC is our model for classified ASC visualization engines," says Louis. The VIEWS team is preparing to deploy gViz, a 64-node cluster designed to support White, with each node consisting of two processors running at 3 gigahertz and sharing one graphics card. Similar clusters are planned to support Purple and BlueGene/L.

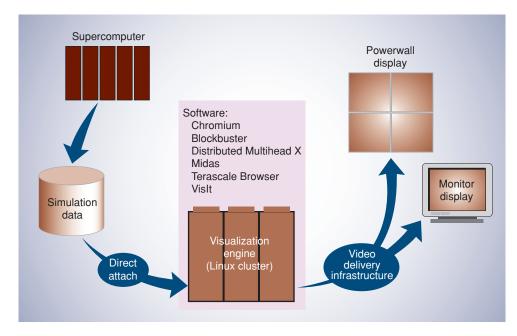
One important advantage of Linux cluster visualization engines is that clusters can be expanded easily. PVC is being tripled in size to support the unclassified demands brought on by Thunder. Similarly, gViz2 is a planned expansion of gViz to either 128 or 256 nodes.

Enormous Software Effort

The VIEWS team has overseen a huge shift in software, which has occurred simultaneously with the development and deployment of new visualization clusters. Many Livermore-developed user applications that ran on the old visualization systems were modified to run on the new clusters. Livermore software developers have also written new software, often with academic and industrial partners, to replace the proprietary software that shipped with the old machines. In one instance, the VIEWS team helped a graphics card manufacturer develop a software driver that allows the company's GPUs to work together in the Linux operating system environment.



The visualization engine gViz is a 64-node Linux cluster designed to support Livermore's White classified supercomputer. Each node contains two microprocessors that share one graphics card. Similar clusters are planned to support the Purple and BlueGene/L machines, which are scheduled to arrive in 2005.



Use of a visualization cluster involves interdependent software and hardware resources, including computational nodes, graphics services, display devices, and video switches.

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The new cluster software is open source, which means that the source code—the software's programming code—is freely available on the Internet through such organizations as SourceForge. "A benefit of this approach is that the public can use our software, make improvements, and notify us if they find any bugs," says Ahern. Although several new software components are being developed under separate projects, many of the developers serve on multiple projects, thereby ensuring that all components work well with each other.

The software component Chromium provides a way for interactive 2D and 3D graphics applications to operate on clusters and allows the applications' graphics cards to work together on a single visualization problem. Ahern and former Livermore computer scientist Randall Frank, in close collaboration with researchers from Stanford University, the University of Virginia, and Tungsten Graphics, designed the software.

Chromium, which won an R&D 100

Award in 2004, supports any program that uses the OpenGL programming language, an industry-standard for drawing graphics. (See *S&TR*, October 2004, pp. 6–7.) Ahern says, "Chromium is a Swiss army knife of graphics 'tool kits' because it fully exploits a cluster's visualization capabilities."

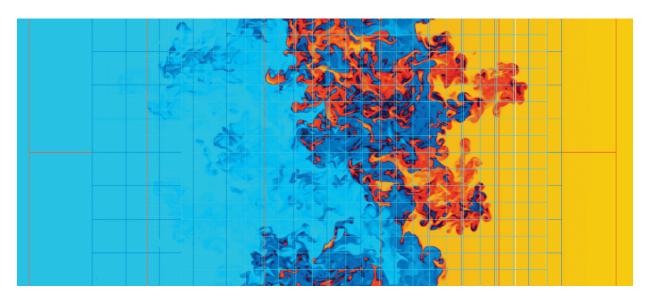
The Distributed Multihead X (DMX) software component combines multiple displays from multiple machines to create a single unified screen. It can create a display from two desktop machines or unify, for example, a 4-by-4 grid of displays (each attached to one of 16 computers) into one giant display. The software is particularly useful for powerwalls. DMX is bundled by Red Hat with its Linux software and is available as open-source software.

Physicists in Livermore's Defense and Nuclear Technologies (DNT) Directorate use Livermore's VisIt software tool to view extremely large scientific data sets. They can animate and manipulate the visualizations and save them as images for presentations. VisIt has been modified to run on the new Linux clusters, and it is freely available.

Livermore's Terascale Browser, a complementary program to VisIt, is another interactive tool that handles extremely large data sets and generates movies from the data. VIEWS developers are working on new ways for users to look for interesting areas with a coarser resolution and then zoom in with higher resolution to view the areas in finer detail.

Another Livermore program, MIDAS, permits visualizations of large simulations to run on office desktop monitors. MIDAS compresses images to one-tenth their original size without sacrificing the detail on the user's display.

Two tools, Telepath and Blockbuster, streamline the process of using large displays. Telepath orchestrates a visualization session by automating the configuration of all the resources required for showing advanced simulations.



Researchers used the RAPTOR code to generate the data used by the software tool Visit to create this two-dimensional image on the Production Visualization Cluster. The image shows the density differences between two gases mixing, which is caused by multiple shock-wave accelerations. The dense gas (sulfur hexafluoride) is depicted in gold, and the light gas (air) is depicted in light blue. The intermediate colors (darker blue to red) denote the mixing of the two gases on a small spatial scale. Overlaid on the figure is a grid that represents the data at increasingly finer spatial and temporal resolutions.

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"Telepath greatly simplifies things for users," says Ahern. Blockbuster, developed for clusters, plays high-resolution movies at 30 frames per second on powerwalls and other large displays.

Combing through a Billion Zones

As simulations grow in size, the ability of users to visually inspect their data has become increasingly limited. "We want to reduce the amount of information users must interact with so they can focus on the most useful details," says Louis. "It would take months to look at all the data. We need ways to drill down and find the most important subsets."

Livermore physicist Steve Langer studies how a laser beam interacts with a 2-millimeter-diameter stream of plasma. His simulations use a mesh composed of 12.7 billion zones, each of which depicts a different region of space. "That's an enormous amount of information," says Langer. "We can't manually inspect 12.7 billion zones to find the ones in which interesting events are occurring."

Given the sheer volume of data, computer science researchers need to help tease out the most relevant features. For example, Sapphire, a Livermore project, attempts to extract underlying patterns in a simulation. This research and development effort taps the field of data mining, which is the process of extracting useful information from raw data. The effort, led by Chandrika Kamath and funded by the Laboratory Directed Research and Development Program, uses such techniques as image processing and pattern recognition. Sapphire techniques are being applied to DNT data both to explore simulation results and to compare these results with experiments. (See *S&TR*, September 2000, pp. 20–22.)

The SimTracker data management tool helps scientists cope with organizing large amounts of simulation data using automated summaries. This tool, which originated at Livermore, has also been adopted by other national laboratories to archive, annotate, and share data. SimTracker summaries

allow users to easily access data analysis tools while browsing graphical snapshots, input and output files, and associated information, all tied into one convenient Web-based collection.

In addition to SimTracker, tools have been developed to automate manual data management processes and simplify the user interface to data. When combined with the suite of hardware and software visualization tools, these data management tools provide ASC users with what they need to manage, analyze, and present their data.

Verdict: Fast, Very Fast

The nearly unanimous opinion about the new Linux clusters is strong approval,

if not downright devotion. "Users are impressed with the clusters," says computer scientist Hank Childs, who helps DNT physicists visualize complicated simulations on PVC for unclassified, stockpile stewardship—related work. "It's a night-and-day difference between the clusters and the older shared-memory visualization engines. Visualization programs run 10 times faster."

Ahern notes that the increased computational horsepower of the Linux clusters allows users to run larger simulations in the same amount of time and display simulations with greater resolution. Langer notes that the clusters are proving themselves especially adept at rotating images faster than the old machines.



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Collaborations Key to Visualization Advances

In many respects, partnerships are key to the continuing success of the National Nuclear Security Administration's (NNSA's) Advanced Simulation and Computing (ASC) Program. For example, NNSA managers and IBM and Livermore computer scientists have collaborated on the design of increasingly more powerful supercomputers.

The Academic Strategic Alliances Program, an ASC program, engages the best minds in the U.S. academic community to help advance simulation science. That goal is shared by Livermore's Institute for Scientific Computing Research. Each year, the institute brings visiting postdoctoral researchers, faculty, and graduate students to the Laboratory. It also hosts an increasing number of undergraduate students majoring in computer science, who participate in computer programming internships.

Most visitors are integrated into the Center for Applied Scientific Computing (CASC), the research arm of Livermore's Computation Directorate, where they work on high-profile research projects. CASC has long-term visualization research relationships with the University of California (UC) at Davis, Duke University, Georgia Institute of Technology (Georgia Tech), University of North Carolina at Chapel Hill, University of Utah, and Stanford University.

Many people first become acquainted with Livermore visualization research at Laboratory-sponsored workshops. "We sponsor workshops so that a number of knowledgeable people can gather to think through issues, such as what it takes to support a 100-teraops machine," says computer scientist Mark Duchaineau, who oversees many students working in CASC.

Duchaineau notes that visiting faculty and students gain valuable experience by working with some of the world's most powerful supercomputers. "There's an atmosphere here that is hard to duplicate at other institutions," says Duchaineau. "Visiting students and faculty become part of the big science we do here. They have access to some of the best equipment in the world, and they assist us with visualizing such phenomena as material properties, shock waves, hydrodynamics, radiation transport, and astrophysics. Our research team publishes extensively, and that's good for people's careers."

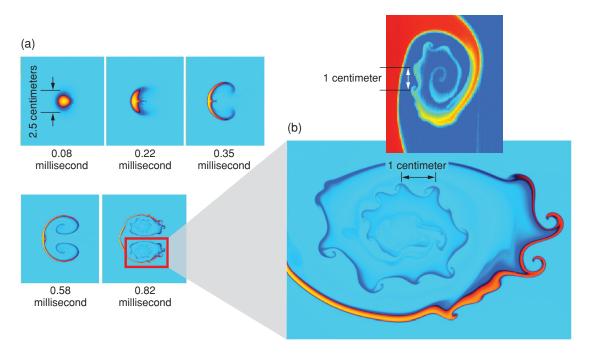
Computer scientist Daniel Laney obtained his Ph.D. from the UC Davis Department of Applied Sciences at Livermore. Laney's thesis, completed at CASC, focused on novel ways to compress data. He chose Livermore because of the variety of the Laboratory's physics projects and the presence of powerful supercomputers. He is currently working on new ways to model planned experiments on Livermore's National Ignition Facility. "In CASC, we provide the proof of concept and then depend on VIEWS software engineers to make it a practical application for the end user," he says.

Computer scientist Peter Lindstrom works with both students and faculty from Georgia Tech and the University of North Carolina at Chapel Hill, two of the nation's top universities in supercomputing visualization. Both schools also have remote access to some of Livermore's unclassified supercomputers. "The payoff for Livermore," says Lindstrom, "is access to some of the best people in the visualization community."

Computer scientist Mark Duchaineau works in front of a powerwall depicting a lattice of 1 billion copper atoms undergoing enormous strain. Duchaineau helps visiting students and faculty members make the most of their supercomputer visualization research at Livermore.



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(a) These images depict what happens over time when a shock wave accelerates a quantity of sulfur hexafluoride contained in a cylinder diffused with ambient air. The shock wave causes the gas to spiral, and the spirals form tiny unstable vortices. The images were created using the RAPTOR code on the Production Visualization Cluster. (b) The larger image depicts a magnified view of a spiral. The result from an experiment conducted at the University of Arizona (inset) is similar to the simulation result in the larger image.

With plans well under way to bring gViz online and retire the old visualization engines, Louis and other VIEWS managers are looking ahead to purchasing visualization clusters to support Purple and Blue Gene/L. At the same time, computer scientists are searching for ways to make the clusters process data more efficiently. "We know we're not yet taking full advantage of the Linux clusters, especially the graphics cards," says Louis. GPUs are so powerful that the VIEWS team and others are exploring their potential for general-purpose computing.

The VIEWS Program (recently renamed Data and Visualization Sciences) is also seeking a hardware solution to compositing. The compositing process pieces together bits of an image, each done by a separate node, into a whole. Currently performed by software, the

technique could be made faster if done by a specialized card linked to each GPU.

Louis says the many advances taking place in hardware and software are permitting researchers to not only see their simulations in breathtaking detail but also understand them to a much greater degree. The winners are Livermore stockpile stewardship scientists and, ultimately, national security.

-Arnie Heller

Key Words: Advanced Simulation and Computing (ASC) Program, BlueGene/L, Center for Applied Scientific Computing (CASC), Chromium, Distributed Multihead X (DMX), gViz, Linux, Purple, stockpile stewardship, supercomputing, Terascale Browser, Visual Interactive Environment for Weapons Simulation (VIEWS), VisIt, White.

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The Right Bang for the Job

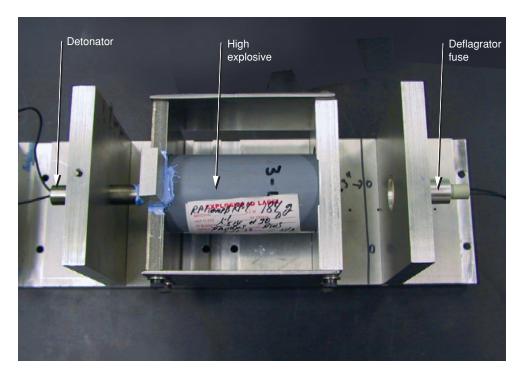
WHEN you think of hand grenades, perhaps the first thing that comes to mind is a classic World War II (WWII) movie scene with a John Wayne—type hero leading his troops up a hill. At the top of the hill, the hero drops to his belly, pulls the pin from a hand grenade, and pitches it into an enemy bunker. Fast-forward half a century and warfare has changed dramatically, shifting from classical battlefields to urban conflicts that call for different tactics and armaments. The hand grenade, however, has remained largely unchanged.

Typically, U.S. soldiers are issued onesize-fits-all grenades to use in a variety of conflict environments and situations. This standard-issue grenade has a kill radius of about 5 meters and is designed for use against small fortifications and small groups of combatants. However, in some urban combat situations, this standardissue grenade could be too powerful and could injure civilians and the soldiers using the grenades.

In recent years, U.S. soldiers have been increasingly engaged in urban warfare. These combat settings may have targets far different from a WWII-type machine-gun

nest. Targets may include enemy quarters or weapons stockpiles housed in buildings set close to active civilian centers, such as schools, water facilities, or buildings of cultural or religious value. Combat situations also have become increasingly complicated. For example, a soldier may need to target a roomful of enemy combatants located next door to a roomful of hostages.

Imagine if a soldier could tailor a grenade's explosive force to the job at hand. With the turn of a dial, the soldier could set the kill radius of the grenade to a distance less than 5 meters and demolish the target while leaving civilians and nearby structures unscathed. Bill Bateson, a Livermore computational physicist at the Center for Applied Scientific Computing (CASC), has been designing such an adaptable hand grenade. The Laboratory's Defense and



Photograph of the experimental apparatus used to test a yield-select hand grenade. A PVC cylinder the size of a soda can (center) is packed with a high explosive commonly used in grenades. A deflagrator fuse is attached to one end of the cylinder (right), and a detonator fuse is attached to the opposite end (left). A "witness" steel plate is used to seal the aluminum apparatus and measure the amount of damage done by the explosion.

Nuclear Technologies (DNT) Directorate is funding the project through discretionary spending.

Using Deflagration to Tailor a Yield

In a departure from the conventional grenade design, Bateson proposes adding a deflagrator to burn a preselected amount of high explosive (HE) before the detonator is set off. The concept is based on an idea that a grenade's burning of HE can be separated into two phases—a deflagration (quick-burning) phase that first consumes HE followed by the standard detonation (rapid-explosion) phase. The burning of HE during deflagration would lead to a less violent reaction and, thus, less destruction than would be caused by a full-yield explosion.

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The seed for yield select was planted when Bateson—not usually a weapons designer—was doing computational modeling of conventional HE. "I was playing with ideas," says Bateson. "How does HE work? How does one get it to detonate? How does one get it to deflagrate? I thought of experiments that could help us understand how HE works." Later, in a conversation with an Army colonel, Bateson recognized the need for yield selection. "I realized that Livermore could provide this technology." Management in both CASC and DNT agreed that developing yield-select technology could benefit the Laboratory and, in a cooperative effort, gave Bateson the go-ahead.

Proving the Principle

To date, Bateson has demonstrated proof of principle with a contraption that simulates a grenade. A PVC cylinder about the size of a soda can is packed with Comp-B, which is an HE commonly

used in grenades. A deflagrator fuse is attached to one end of the cylinder, and a detonator fuse is attached to the opposite end. This assembly is fitted into an aluminum apparatus the size of a shoe box to which a diagnostic "witness" plate of steel is attached to seal the apparatus. The witness plate is used as a measure of the amount of damage done by the explosion. The assembly is then set to detonate after a predetermined time delay that allows for the deflagration reaction. During that time delay, the excess HE burns in the deflagration phase, leaving less explosive for the detonation phase.

Bateson has experimented with varying detonation time delays following deflagration. He also has achieved full deflagration in which no detonation occurs and full detonation in which there is no time delay for deflagration. The witness plates tell the story of the varying degrees of deflagration. At full deflagration, where no explosion is expected because

the entire HE has burned, the witness plate appears unscathed. At full detonation, however, the plate is considerably damaged and has a characteristic angled bend exhibited by all plates from experiments involving a detonation. As expected, witness plates from explosions set for longer deflagration phases show less damage and bend.

The idea of yield select is not new. Researchers have been pondering possible designs for some time. One of the design challenges has been to initiate the deflagration reaction, while preventing the HE from detonating. Bateson overcame this obstacle with one small modification to a detonator fuse. The detonator is a shaped-charge explosive train, which means it has a liner between the initiating explosives and the main charge. The liner forms a "jet" when the initiating explosives (PETN and RDX) ignite. These initiating explosives launch the jet into the HE (Comp-B) in the grenade cylinder, which causes the

HE to ignite. The liner in a standard detonator is made from copper, which triggers detonation. Bateson reasoned that if the copper liner were substituted with another material, deflagration could be achieved. Hence, the detonator could be used as a deflagrator. Indeed, when this theory was tested, the modified shaped-charge fuse created a jet that set off a deflagration instead of a detonation when it hit the Comp-B.

Just Getting Started

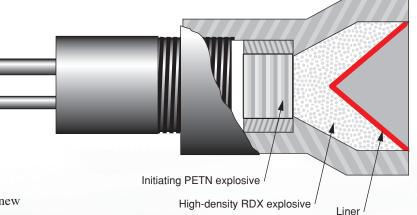
Despite the early success and excitement about yield select, much more work is needed to refine the system. "We're in the first stages of design," says Bateson. "People are asking if we can design a handheld-size yield-select grenade. The answer is yes." Bateson sees size-slimming opportunities for both the deflagrator fuse and detonator fuse. By trimming down these fuses a few centimeters each, the yield-select hand grenade could be close to the size of currently manufactured



The steel "witness" plates show the range of effects from full deflagration (left) to full detonation (right) of a yield-select grenade.

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This schematic shows the newly designed deflagration fuse, which is a shaped-charge explosive train.



hand grenades. These new grenades would fit into existing grenade casings, shortening the time required to advance the new technology into the field.

The corollary to the size question is how scalable is yield select? "The Air Force wants a 2,000-pound yield-select bomb," says Bateson. "Now, the question is how do we scale up from a hand grenade? Do we use one large deflagrator or a chain of smaller deflagrators?"

In a recent directive to the secretaries of all military branches, the Office of the Secretary of Defense (OSD) stated that in the continuing pursuit of reducing collateral damage to civilians and civilian structures, all current ammunitions are to be considered for yield-select capability. "The OSD wants anything that hits the ground—bombs, grenades, mortars, rockets, or artillery shells—to be yield select," says Bateson." Clearly, the demand for yield select is big.

-Maurina S. Sherman

Key Words: ammunition, collateral damage, deflagration, detonation, hand grenade, high explosives (HE), yield select.

For further information contact Bill Bateson (925) 422-9047 (bateson1@llnl.gov).

Cell by Cell: Moving Biology toward a More Predictive Future

OR years, physicists and chemists at the Laboratory have reaped the benefits of the versatility and power of computer codes designed to study the physical and chemical processes underlying high-explosives detonations. Now, biologists are also looking to computer codes for understanding the intricate processes underlying cellular reactions.

A growing interest exists within Livermore's Biology and Biotechnology Research Program (BBRP), and the biology community, to pursue "quantitative biology." This emerging discipline, targeted at the understanding of biological processes, will integrate experimental data into predictive models that harness the same computational power used by physicists and chemists. Computational results can, in turn, be used to design and evaluate new experiments.

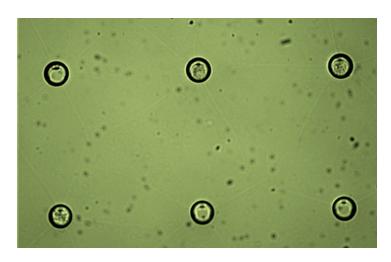
BBRP is taking on a new initiative to develop a system for gathering massive amounts of individual cellular data. These data will be used to help build computational models of cells, which, in turn, will help scientists achieve a quantitative understanding of the cellular life cycle. "Computational modeling offers many benefits that biologists hope to apply in guiding experiments and understanding the results of research efforts," says Livermore biologist Allen Christian. "The thrust of this effort is the gathering of quantitative cellular measurements for input into computer codes. The codes can then be used to model how cells react to various environments and to different stimuli or disturbances."

Piecing together cellular processes helps scientists gain an understanding of stepwise cellular pathways, enabling them to predict cellular reactions. This knowledge could lead to the discovery of new technologies ranging from drug therapies to protection against bioterror attacks.

Gathering the Data to Feed the Codes

Sophisticated computer modeling provides the framework to help design experiments. With computer modeling, hypotheses can be developed and testable predictions made. Currently, computer codes are being used at Livermore to study cell signaling through the calcium ion channels between epithelial cells. (See *S&TR*, January/February 2003, pp. 15–18.) Codes such as these represent a first step toward the more comprehensive goal of quantifying a library of myriad cellular processes.

One of the greatest challenges biologists face in developing biological computer models is the need for precise data on the



In the instrumented cell system, a microchip is designed to capture, sustain, and experiment on a single cell. Each circular capture well is approximately 10 micrometers across and contains a single human cancer cell.

concentration and distribution of cellular components, such as nuclei and mitochondria. However, gathering the massive data necessary to feed a useful code is much more difficult for biologists than for their physicist and chemist counterparts. For the most part, first principles can be used in physics and chemistry to supply consistent and reliable data. Biology is different. Although the cell—the basic unit of life—can be generally characterized, each individual cell reacts differently than its neighbor when picked and prodded with an experimental disturbance—be it a pathogen, enzyme, electrical current, optical interference, or some other disruption. And the information collected in conventional experiments that aggregate in one sample the data from many cells simply isn't sufficient for computational modeling. To be useful in a computer code, data must reflect the diverse conditions found in individual cells.

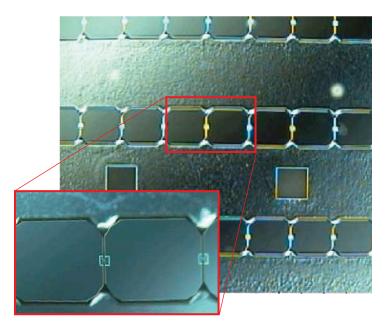
Mike Colvin, a computational biologist whose work has advanced the idea of a system capable of taking individual cell measurements, explains that a number of phenomena prevent the accurate representation of cellular processes when using pooled or aggregate data. "We lose information about what individual cells are doing," says Colvin. For example, conventional experimental techniques, such as pooling dissolved cells, destroy data about a

cell's location. Colvin also points out that many biologic processes create asymmetries at the cellular level. While these variable properties may not be accurately reflected in pooled data, single-cell measurements can provide averages and reflect variance in cellular processes. Thus, quantitative data from individual cells are essential to create accurate and reliable computational models that can lead researchers to a predictive understanding of cellular pathways.

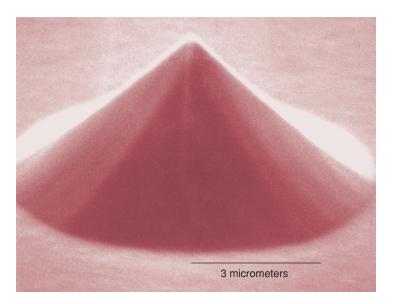
New System Speeds Accurate Cellular Measurement

For the Department of Energy's Genomics:GTL (formerly Genomes to Life) Program, the development of an "instrumented cell" system is expected to be the enabling technology that kick-starts the data gathering. With funding from the Laboratory Directed Research and Development (LDRD) Program, Christian's group is creating an instrumented cell system that allows high-throughput measurement of individual cells. Studies of specific cellular responses require the ability to index cells in a way that preserves their identity during an experiment. Christian's group envisioned the configuration of an array of individual cells, each fixed in a specific location. This idea led to the development of a microchip that Christian and his team have fabricated to capture, sustain, and experiment on individual cells.

The microchip consists of wells that are just the right size to hold only one cell. Because cells vary considerably in size, the



This image shows a microchip with arrays of capture wells that are small enough to trap individual bacteria. The inset is a magnified view of a single well, which is located in the vertical space between two adjacent rectangular bases. In the space is a narrow gap where a bacterium is trapped as the flow is drawn through.



A Livermore-designed glass microneedle will be manufactured in arrays and used to inject and sample large numbers of captured cells at once. This manipulation technology, combined with the technology for capturing and maintaining cells, will ensure the high throughput necessary to produce large amounts of data quickly.

microchip will eventually be made with interchangeable wells. Single cells are captured in the wells by first flowing a liquid containing the cells onto the chip. A syringe pump then pulls the liquid through an opening in the bottoms of the wells, which are small enough to trap the cells inside.

Keeping the cells alive after capture is one of the project's greatest challenges—and what makes this capability unique in the world. The liquid environment in which the cells are maintained amounts to an artificial blood stream that must deliver nutrients and maintain the proper level of carbon dioxide and a temperature of 37°C, among other variables. The slightest deviation in any of these variables from what the cell is accustomed to can cause the cell to behave differently—which would defeat the purpose of studying the response of cells under normal conditions.

The team is also fabricating glass microneedles for injecting substances into the captured cells and sampling their interior. The needle will be fabricated in arrays corresponding to the position of each cell-capture well in order to inject multiple cells at once. The ability to simultaneously capture and manipulate large numbers of cells will ensure the high throughput necessary to produce large amounts of data quickly. The team is also writing software to automate the entire process, further enhancing the accuracy of analysis and reducing costs.

The instrumented cell system can be fitted with standard measurement and imaging instruments, such as infrared

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spectroscopes, fluorescence microscopes, and bright-field microscopes. The system is currently capable of arraying large numbers of human cells, but plans are in place to expand its use to bacterial cells.

A Systems Approach to Biology

"The whole field of biology is moving toward systems biology, whether that system be one cell or an entire organism or environment," says Colvin. With the completion of the Human Genome Project, scientists have a rich understanding of the genome and many of the proteins constructed by genes. Much is known about biochemical pathways and intracellular transport. The workings and functions of organs and organelles are well understood. However, despite the enormous amount of knowledge gleaned about myriad pathways, biochemicals, enzymatic reactions, cellular receptors, ion channels, protein—protein interactions, and so forth, little is known about how all these units work together as a system.

By breaking down living organisms into manageable units, researchers have been able to study individual parts—indeed parts of parts. This effort has led to the mapping of many cellular pathways, but few quantitative data have come from it. New techniques such as computational modeling are now helping biologists to develop a systems approach to understanding and predicting cellular processes. The challenge is to gather the

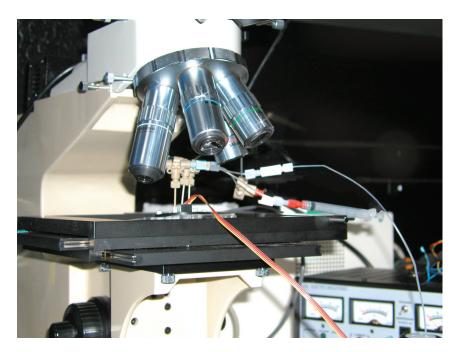
massive amounts of data necessary to feed computational codes that are so extraordinarily complex, they simulate life.

Integrating the System with Gene-Silencing Technology

Christian plans to combine the new instrumented cell system with his group's award-winning siHybrid gene-silencing technique, which thwarts gene expression by inserting short interfering RNA–DNA hybrid molecules into cells. (See *S&TR*, October 2004, pp. 10–11.) The recently developed siHybrids, funded by LDRD, enable the robust study of how genes create proteins and how those proteins function. The siHybrids will help generate some of the key data to be quantified using the instrumented cell system.

The instrumented cell effort is expected to spawn breakthroughs in many Laboratory- and DOE-relevant biological applications, including improved explication of the DNA-repair system, the elucidation of host-pathogen interactions, and the understanding of microbial communities. Colvin points to the Laboratory's analytic and computational capabilities as strengths that can establish Livermore as a leader in this new era of biology. Core technologies that have been developed for other applications, such as microfabrication, advanced imaging, and mass spectrometry, will help the Laboratory play a leading role in moving biology from what many consider a descriptive science to a quantitative and, ultimately, predictive science.

-Maurina S. Sherman



The instrumented cell system can interface with standard imaging and measurement instruments, such as microscopes and spectroscopes.

Key Words: Biology and Biotechnology Research Program (BBRP), cellular processes, computational biology, Genomes to Life, genomics, GTL:Genomics, Human Genome Project, instrumented cell, Laboratory Directed Research and Development (LDRD), microfluidics, quantitative biology, systems biology.

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Each month in this space, we report on the patents issued to and/or the awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patents

Ergonomic Material-Handling Device

Lance E. Barsnick, David M. Zalk, Catherine M. Perry, Terry Biggs, Robert E. Tageson

U.S. Patent 6,779,803 B1

August 24, 2004

A handheld ergonomic material-handling device helps move heavy objects requiring mechanical assistance, such as large waste containers. The device allows users to move a heavy object while keeping their back, shoulders, wrists, and knees in a neutral posture, thereby reducing potential injury. One key feature of the device is handles with adjustable heights to fit a user's back, wrists, and shoulders. Another key feature is the rounded shape of the handlebar, which keeps a user's wrists in a neutral posture during manipulation of the device.

Magnetohydrodynamic Fluidic System

Abraham P. Lee, Mark G. Bachman

U.S. Patent 6.780.320 B2

August 24, 2004

This magnetohydrodynamic (MHD) fluidic system includes a reagent source containing a reagent fluid and a sample source containing a sample fluid and a constituent. A reactor is connected to the reagent and sample sources. The MHD pump uses a drive to move the reagent and sample fluids. This flow allows the reagent and sample fluids to form an interface causing the constituent to be separated from the sample fluid.

Apparatus for Improving Performance of Electrical Insulating Structures

Michael J. Wilson, David A. Goerz

U.S. Patent 6,783,401 B2

August 31, 2004

This apparatus removes the electrical field from the internal volume of high-voltage structures (for example, bushings, connectors, capacitors, and cables). The electrical field is removed from the inherently weak regions of the interconnect, such as between the center conductor and the solid dielectric, and is placed in the primary insulation. This is accomplished by providing a conductive surface on the inner surface of the principal solid dielectric insulator that surrounds the center conductor. The center conductor is connected to this conductive surface. The advantage of removing the electrical fields from the weaker dielectric region to a stronger area is improved reliability, increased component life and operating levels, reduced noise and losses, and a more compact design. This electrical field control approach is currently possible on many existing products at a modest cost. Several techniques are available to provide the level of electrical field control needed. Choosing the optimum technique depends on material, size, and surface accessibility. The simplest deposition method uses a standard electroless plating technique. Other metallization techniques include vapor and energetic deposition, plasma spraying, conductive painting, and other controlled coating methods.

Rolling Circle Amplification Detection of RNA and DNA

Allen T. Christian, Melissa S. Pattee, Cristina M. Attix, James D. Tucker U.S. Patent 6,783,943 B2

August 31, 2004

Rolling circle amplification (RCA) has been useful for detecting point mutations in isolated nucleic acids, but its application in cytological preparations has been problematic. By pretreating cells with a combination of restrictive enzymes and exonucleases, we can demonstrate RCA in solution and in situ to detect gene copy number and single-base mutations. RCA is also useful for detecting and quantifying transcribed ribonucleic acid in individual cells, making it a versatile tool for cell-based assays.

Target Molecules Detection by Waveguiding in a Photonic Silicon Membrane

Sonia Letant, Anthony Van Buuren, Louis Terminello

U.S. Patent 6,785,432 B2

August 31, 2004

This waveguiding photonic silicon filter can bind and detect biological and chemical target molecules in liquid or gas samples. The filter has chemical or biological anchors covalently attached to its pore walls and selectively binds target molecules. Transmission curve engineering principles allow in situ and real-time measurements to detect the presence of various target molecules and determine the concentration of bound target.

Dielectrophoretic Concentration of Particles under Electrokinetic Flow Robin R. Miles, Kerry A. Bettencourt, Christopher K. Fuller

U.S. Patent 6,787,018 B1

September 7, 2004

Dielectrophoresis is used to collect particles under the conditions of electrokinetically driven flow. Interdigitated electrodes are patterned on an inner surface of a microfluidic channel. A direct current voltage is applied across the ends to the channel, and an alternating current voltage is applied across the electrodes. Particles swept down the channel electrokinetically are trapped within the field established by the electrodes. The particles can be released when the voltage to the electrodes is released.

Detection and Treatment of Chemical Weapons and/or Biological Pathogens

Raymond P. Mariella, Jr.

U.S. Patent 6,787,104 B1

September 7, 2004

A system for detecting and treating chemical weapons or biological pathogens uses a detector assembly, an electrostatic precipitator or scrubber, a circulation system, and a control. The precipitator or scrubber is activated in response to a signal from the detector when it detects chemical weapons or biological pathogens.

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High Energy Laser Beam Dump

John Halpin

U.S. Patent 6,792,017 B2

September 14, 2004

The laser beam dump is positioned in a housing. An absorbing glassplate means is operatively connected to the housing. A heat-sync means for extracting heat from the absorbing glass-plate means is operatively connected to the housing and the absorbing glass-plate means.

Multi-Stage Combustion Using Nitrogen-Enriched Air Larry E. Fischer, Brian L. Anderson

U.S. Patent 6,790,030 B2

September 14, 2004

Multistage combustion technology is combined with nitrogen-enriched air technology to control combustion temperature, extend the maintenance and lifetime cycles of materials in contact with combustion products, and reduce pollutants while maintaining relatively high combustion and thermalcycle efficiencies. The first stage of combustion operates fuel rich as most of the combustion heat is released with the burning of nitrogen-enriched air. Part of the energy in the combustion gases is used to perform work or to provide heat. The cooled combustion gases are reheated by additional stages of combustion until the last stage is at or near stoichiometric conditions. Additional energy is extracted from each stage to result in relatively high thermal-cycle efficiency. The air is enriched with nitrogen using air-separation technologies, such as diffusion, permeable membrane, absorption, and cryogenics. The combustion method can be used with many types of combustion equipment, including boilers, burners, turbines, and internal combustion engines. Many types of fuel can be used with this method, including hydrogen and carbon-based fuels.

DC Attenuation Meter

Douglas L. Hargrove

U.S. Patent 6,791,337 B2

September 14, 2004

A portable, handheld meter measures direct current (dc) attenuation in low-impedance electrical signal cables and attenuators. A dc voltage is applied to the signal input of the cable and to feedback from the control circuit through the signal cable and attenuators. The control circuit adjusts the applied voltage to the cable until the feedback voltage equals the reference voltage. The units of applied voltage required at the cable input equals the system attenuation value of the cable and attenuators, which makes this meter unique. The meter may be used to calibrate data-signal cables, attenuators, and cable-attenuator assemblies.

Differentially-Driven MEMS Spatial Light Modulator

Eddy A. Stappaerts

U.S. Patent 6,791,735 B2

September 14, 2004

A microelectromechanical system (MEMS) spatial light modulator (SLM) and an electrostatic actuator associated with a pixel in an SLM. The actuator has three electrodes: a lower electrode, an upper electrode fixed with respect to the lower electrode, and a center electrode suspended and actuable between the upper and lower electrodes. The center electrode is capable of resiliently biasing to restore the center electrode to a nonactuated first equilibrium position. A mirror is operably connected to the center electrode. A first voltage source provides a first bias voltage across the lower and center electrodes, and a second voltage source provides a second bias voltage across the upper and center electrodes. The first and second bias voltages determine the nonactuated first equilibrium position of the center electrode. A third voltage source provides a variable driver voltage across one of the lower–center and upper–center electrode pairs, in series with the corresponding first or second bias voltage, to actuate the center electrode to a dynamic second equilibrium position.

High Average Power Scaling of Optical Parametric Amplification through Cascaded Difference-Frequency Generators

Igor Jovanovic, Brian J. Comaskey

U.S. Patent 6,791,743 B2

September 14, 2004

A first pump pulse and a signal pulse are injected into a first optical parametric amplifier. This method produces a first amplified signal pulse. At least one additional pump pulse and the first amplified signal pulse are injected into at least one additional optical parametric amplifier, producing a higher power coherent optical pulse.

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Awards

In June 2004, the U.S. Air Force honored **Bruce Goodwin**, **George Sakaldasis**, and **Larry Altbaum** each with the **Exemplary Civilian Services Medal**. This medal is the highest Air Force civilian service award and is equivalent to the military's Distinguished Service Medal. Goodwin is associate director for Defense and Nuclear Technologies, Sakaldasis is assistant director for Military Affairs in the Laboratory's National Security Office, and Altbaum leads the Weaponization Program in the Defense Technologies Engineering Division.

Theodore Saito received the Exceptional Public Service

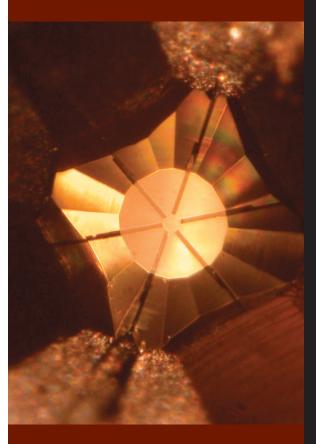
Award from the Department of Defense (DoD) for his work in nonproliferation policy at the Pentagon from September 2002 to June 2004. Saito, a senior staff engineer who has worked at the Laboratory for 20 years, was assigned to work in Washington, DC, for the Department of Energy in September 2001 as the scientific advisor for the National Ignition Facility. A year later, he was transferred to the Pentagon in a DoD-sponsored position working with the offices of Non-Proliferation Policy and Short-Arms-Control Policy. Additionally, Saito served as the lead officer on the Comprehensive Nuclear Test Ban Treaty and helped draft Senate testimony adding protocol language to the treaty. He also collaborated with the International Atomic Energy Agency and was instrumental in the federal government's efforts to monitor nuclear weapons in foreign nations such as India, Pakistan, Iran, and South Korea.

In August 2004, **John Wolf**, a radiological characterization analyst, received one of the top awards at the national meeting

of the Academy of Certified Hazardous Materials Managers (ACHMM) in Las Vegas, Nevada. Wolf earned the **Young CHMM of the Year Award** for his outstanding contributions and significant accomplishments in the hazardous materials management, environmental, and health and safety fields. This award was given to Wolf as the brightest and best of young (35 years or younger) CHMM professionals. In addition, Wolf received a **Champion of Excellence Award** for his promotion of the CHMM credential and professional development activities as president of the Northern California Chapter. ACHMM is a national organization with more than 6,000 certified professionals supporting environmental and waste management programs, projects, and activities in the U.S.

Plant Engineering's Permit Office and Damage
Prevention Team has been awarded the Government Video
Star Award for its training video entitled "Soil Excavation
and Concrete Penetration Permit Process and Awareness at
Lawrence Livermore National Laboratory." Both Laboratory and
subcontractor employees performing excavation and concrete
penetrations at Livermore are required to review the video
prior to performing work. The Government Video Technology
Exposition is the East Coast's largest conference and exposition
created exclusively for government communication professionals
and their specific product and service needs. The team's work
was recognized at the Seventh Annual Government Video
Technology Exposition during a ceremony on October 6, 2004, in
Washington, DC.

Diamonds Put the Squeeze On



A new type of diamond anvil cell encapsulates tiny wires in a thin diamond film to reveal information about materials under high pressure.

Also in December

- The Critical Assessment of Structural Proteins experiment helps scientists evaluate which methods best predict protein structure.
- Detailed simulations of fluids help physicists better understand systems in motion.
- Livermore's high-flux radiography system allows scientists to observe a detonating material.

Probing the Universe with Mirrors That Trick Light

Livermore researchers have developed high-energy x-ray focusing optics for many applications, including astrophysics, medical imaging, laser target characterization, and radiation detection for homeland security. Recent developments in multilayer optics and high-atomic-number (high-Z), solid-state pixel detectors now make both focusing optics and detectors possible at high x-ray energies. Laboratory researchers are collaborating on the High Energy Focusing Telescope (HEFT), a balloon mission to focus and measure celestial x rays at energies above 20 kiloelectronvolts. HEFT will provide dramatic improvements in sensitivity and angular resolution over previous instruments and allow x-ray observations of supermassive black holes, stars, and pulsars. The Laboratory is also developing x-ray optics for the Small Animal Radionuclide Imaging System, which will allow biomedical researchers to observe the effectiveness of a medical treatment or how well a drug controls DNA damage or carcinogenesis. X-ray optics may also prove valuable for target characterization and imaging at the National Ignition Facility, where it will be important to verify nondestructively that microscopic parts are assembled correctly and are not damaged. Contact:

Bill Craig (925) 423-1471 (craig1@llnl.gov).

From Seeing to Understanding

Extraordinarily complex, three-dimensional (3D) supercomputer simulations play an essential role in making sure the nation's nuclear stockpile remains safe and reliable. Understanding these simulations depends, to a great extent, on the human eye to scrutinize the vast amounts of simulation information translated into still and moving images. The Visual Interactive Environment for Weapons Simulation (VIEWS) Program, part of the National Nuclear Security Administration's Advanced Simulation and Computing Program, is helping Laboratory scientists visually explore, manage, and analyze data from advanced simulations. The Livermore VIEWS team is developing new ways to see and understand the latest simulations by combining inexpensive and ubiquitous microprocessors, graphics cards favored by gaming fans, and open-source software into powerful visualization engines that turn reams of data from supercomputers into viewable 3D images and movies. The team is transitioning visualization engines from proprietary shared-memory designs to groups or "clusters" of commercial microprocessors and high-end graphics cards found in gaming boxes and many desktop computers. When combined with a high-speed network, the Linux operating system, and software tools written in open-source code, the clusters outperform the larger, more expensive, proprietary machines.

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